

Weiss oscillations in the electronic structure of modulated graphene

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Abstract. We present a theoretical study of the electronic structure of modulated graphene in the presence of a perpendicular magnetic field. The density of states and the bandwidth for the Dirac electrons in this system are determined. The appearance of unusual Weiss oscillations in the bandwidth and density of states is the main focus of this work.

PACS numbers: 72.20.My, 72.80.Rj, 73.50.Dn, 73.40.-c

Submitted to: *J. Phys.: Condens. Matter*

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1. Introduction

There has been considerable interest in understanding the electronic properties of a single layer of graphene ever since its experimental realisation. Experimental and theoretical studies have shown that the nature of the quasi-particles in these two-dimensional systems is very different from that of the standard two-dimensional electron gas (2DEG) which has been extensively studied. Graphene has a honeycomb lattice of carbon atoms. The quasi-particles in graphene have a band structure in which electron and hole bands touch at two points in the Brillouin zone. At these Dirac points the quasi-particles obey the massless Dirac equation: they behave as massless particles with a linear dispersion relation $\epsilon_k = vk$ (with the characteristic velocity $v \simeq 10^6 \text{ ms}^{-1}$). This behaviour gives rise to a host of new and unusual phenomena such as anomalous quantum Hall effects and a π Berry phase [1, 2]. This 2D Dirac-like spectrum has been confirmed by measurements of de Haas-van Alphen and Shubnikov-de Haas (SdH) oscillations [3], where magnetic oscillations appear due to the interplay of the Landau levels with the Fermi energy, and are important tools in the investigation of the Fermi surface and electron transport. In a standard 2DEG an artificially created periodic potential in the sub-micron range leads to the appearance of Weiss oscillations in the magnetoresistance. Such electrical modulation of the 2D system can be achieved by depositing an array of parallel metallic strips on the surface or through two interfering laser beams [4, 5, 6]. Weiss oscillations can be explained in terms of the commensurability of the electron cyclotron diameter at the Fermi energy and the period of the electric modulation. These oscillations were found to be periodic in the inverse magnetic field [5, 6, 7]. It is therefore interesting to study the affect on the Dirac electrons of electrical modulation of a graphene layer. In this work we study the effects of modulation on the bandwidth (Δ) and the density of states (DOS) of the Dirac electrons in graphene. These quantities are essential prerequisites for understanding properties such as electron transport, thermodynamic behaviour etc.

In section 2, we present the formulation of the problem. Section 3 contains the calculation of the density of states whereas in section 4 we discuss the bandwidth for electrically modulated graphene including an asymptotic and classical description. The conclusions are in section 5.

2. Formulation

We consider two-dimensional Dirac electrons in graphene moving in the x - y -plane. The magnetic field, $\mathbf{B} = (0, 0, B)$, is applied along the z -direction perpendicular to the graphene plane. This system is subjected to a weak electric modulation along the x -direction. Using the Landau gauge we write the vector potential as $\mathbf{A} = (0, Bx, 0)$. The two-dimensional Dirac like Hamiltonian for a single electron in the Landau gauge is (using $\hbar = c = 1$) [1, 2, 8]

$$H_0 = v\boldsymbol{\sigma} \cdot (-i\nabla + e\mathbf{A}), \quad (1)$$

where $\boldsymbol{\sigma} = \{\sigma_x, \sigma_y\}$ are the Pauli matrices and v is the magnitude of the electron velocity. The complete Hamiltonian of our system may be written as

$$H = H_0 + U(x), \quad (2)$$

where H_0 is the unmodulated Hamiltonian and $U(x)$ represents the periodic modulation along the x -direction modelled as

$$U(x) = V_0 \cos(Kx), \quad (3)$$

where $K = 2\pi/a$, and a and V_0 are the period and amplitude of the modulation respectively. Without modulation the Landau level energies are given by

$$\varepsilon(n) = \omega_g \sqrt{n}, \quad (4)$$

where $\omega_g = v\sqrt{2eB}$ is the cyclotron frequency of the graphene electrons and n is an integer. Note that the Landau level spectrum for Dirac electrons is significantly different from that in a conventional 2DEG where $\varepsilon(n) = \omega_c(n + \frac{1}{2})$ and $\omega_c = eB/m$ is the cyclotron frequency.

The eigenfunctions without modulation are given by [8]

$$\Psi_{n,k_y}(r) = \frac{e^{ik_y y}}{\sqrt{2L_y \ell}} \begin{pmatrix} -i\Phi_{n-1}[(x+x_0)/\ell] \\ \Phi_n[(x+x_0)/\ell] \end{pmatrix}, \quad (5)$$

where

$$\Phi_n(x) = \frac{e^{-x^2/2}}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x), \quad (6)$$

$\ell = (eB)^{-1/2}$ is the magnetic length, $x_0 = \ell^2 k_y$, L_y is the y -dimension of the graphene layer and $H_n(x)$ are the Hermite polynomials.

As we are considering weak modulation such that V_0 is smaller than the Landau level separation we can apply standard perturbation theory to determine the first order correction to the unmodulated energy eigenvalues

$$\Delta E_{n,k_y} = \int_{-\infty}^{\infty} dx \int_0^{L_y} dy \Psi_{n,k_y}^*(r) U(x) \Psi_{n,k_y}(r) \quad (7)$$

with the result [8]

$$\Delta E_{n,k_y} = \frac{1}{2} V_0 \cos(Kx_0) e^{-u/2} [L_n(u) + L_{n-1}(u)] \quad (8)$$

where $u = K^2 \ell^2 / 2$ and $L_n(u)$ are Laguerre polynomials. Hence the energy eigenvalues in the presence of modulation are

$$\varepsilon(n, x_0) = \varepsilon(n) + \Delta E_{n,k_y} = \omega_g \sqrt{n} + |F_n| \cos(Kx_0) \quad (9)$$

with $|F_n| = \frac{1}{2} V_0 e^{-u/2} [L_n(u) + L_{n-1}(u)]$. We observe that the degeneracy of the Landau level spectrum of the unmodulated system with respect to k_y (and x_0) is lifted in the presence of modulation. The formerly sharp Landau levels broaden into bands whose widths, $\sim |F_n|$, oscillate as a function of n since $L_n(u)$ are oscillatory functions of the index n . At this stage we can compare the energy spectrum of Dirac electrons with that of standard electrons in the same system. The differences are:

- the standard electron unperturbed energy eigenvalues depend linearly on both the magnetic field and the quantum number n whereas for Dirac electrons they depends on the square root of both.
- in graphene we have the average of two successive Laguerre polynomials $[L_n(u) + L_{n-1}(u)]/2$ while for standard electrons we have a single term, $L_n(u)$.

These differences will give different results for the density of states and the band width, as we show in the next section. Note that for the weak electric modulation case under consideration the quantum numbers n can be referred to as the magnetic Landau band indices and are equivalent to the Landau level quantum number n for the unmodulated system. In the presence of weak electric modulation, the band width of the magnetic Landau bands depends on the index n . Thus the electric modulation induced broadening of the energy spectrum is non-uniform, a feature which will be of significance in understanding the behaviour of Dirac electrons in modulated graphene.

3. The Density of States (DOS)

It is well known that in the absence of modulation the DOS consists of a series of delta functions at energies equal to $\varepsilon(n)$. The addition of a weak spatially periodic electric modulation, however, modifies the formerly delta function like DOS by broadening the singularities at the energies($\varepsilon(n)$) into bands. The density of states is given by

$$D(\varepsilon) = \frac{1}{A} \sum_{nk_y} \delta(\varepsilon - \varepsilon_{n,k_y}), \quad (10)$$

where the sum on n extends over all occupied Landau levels and A is the area of then sample. By using the energy eigenvalues given in (9), we can express $D(\varepsilon)$ as:

$$D(\varepsilon) = 2 \frac{1}{2\pi a \ell^2} \sum_n \int_0^a dx_0 \delta(\varepsilon - \varepsilon_n - |F_n| \cos(Kx_0)), \quad (11)$$

where $\varepsilon_n = \omega_g \sqrt{n}$, and a factor 2 is due to spin degeneracy. Evaluation of the x_0 -integral in the above equation yields the zero temperature density of states of the modulated two-dimensional Dirac electrons:

$$D(\varepsilon) = \frac{1}{\pi^2 \ell^2} \sum_n \frac{1}{\sqrt{|F_n|^2 - (\varepsilon - \varepsilon_n)^2}} \Theta(|F_n| - |\varepsilon - \varepsilon_n|), \quad (12)$$

where $\Theta(x)$ is the Heaviside unit step function. Here we can see that the one-dimensional van Hove singularities of the inverse square-root type appear at the low and high energy edges of the broadened Landau bands, forming a double peak like structure.

The zero temperature DOS given by (12) is shown graphically in figure 1 as a function of energy, using the following parameters [8]: $v \simeq 10^6 \text{ ms}^{-1}$, $n_D = 3 \times 10^{15} \text{ m}^{-2}$, $a = 350 \text{ nm}$, $V_0 = 0.35 \text{ meV}$, and $k_F = (2\pi n_D)^{1/2}$ being the Fermi wave number of the unmodulated system in the absence of a magnetic field. The origin of both Weiss and of Shubnikov-de Haas (SdH) oscillations is immediately apparent. The short period, high amplitude oscillation is the Landau level structure which gives rise to SdH

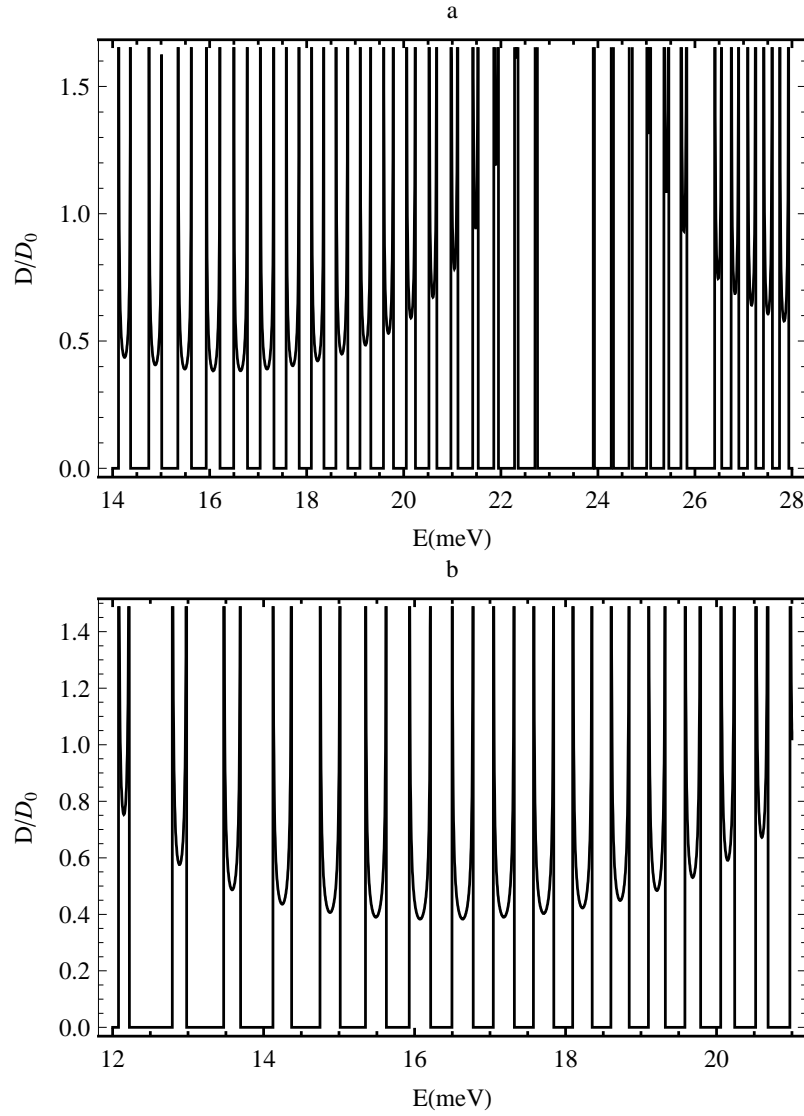


Figure 1. The dimensionless density of states, D/D_0 , in a periodically modulated graphene as a function of energy (a & b have different energy ranges only, all other parameters are the same) for fixed value of magnetic field $B = 0.35$ T.

oscillations whereas the apparent darker longer period oscillation (actually the minima in the DoS for each Landau level) is associated with the Weiss oscillations. This is largely a consequence of the oscillatory factor $|F_N|$, which has been shown to exhibit commensurability oscillations. Our basic density of states spectrum is exactly the same as shown by others [9] without modulation, as is the Weiss period, albeit with an extra modulation.

4. The Bandwidth (Δ)

To better appreciate the modulation of the amplitude of Weiss oscillations we plot the bandwidth as a function of the magnetic field in figure 2. The width of the n^{th} Landau level is given as

$$\Delta = 2 |F_N| = V_0 \exp^{-\frac{u}{2}} |L_n(u) + L_{n-1}(u)| . \quad (13)$$

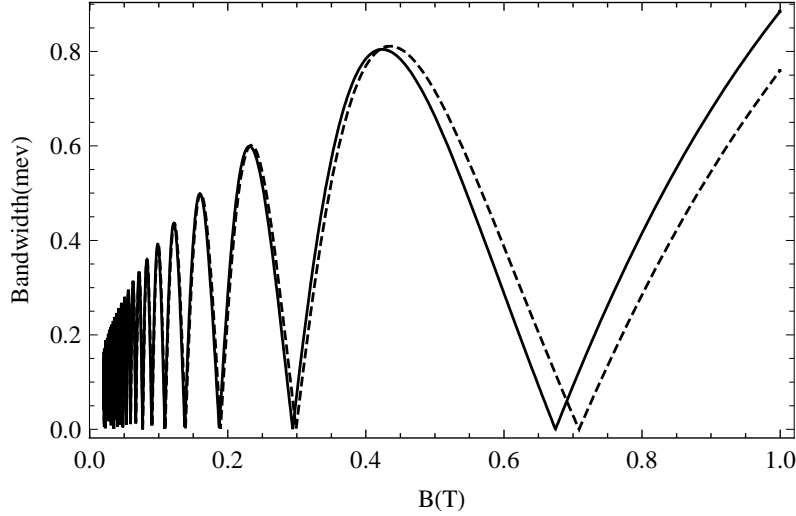


Figure 2. Bandwidth due to periodic electric modulation 2D graphene as a function of magnetic field. The dotted line is the asymptotic behaviour and solid line represents the exact behaviour of the width.

This is clearly different from the standard electron result [4, 5, 6]. The bandwidth is plotted for $n = n_F$ where $n_F = E_F^2/\omega_g^2$ is the Landau level index at the Fermi energy. Contrast this with $n_F = E_F/\omega_c - \frac{1}{2}$ and $\omega_c = eB/m$ for a standard 2DEG. For the low magnetic fields under consideration, the graphene results for Dirac electrons are the same in phase and amplitude as those for standard electrons. Moreover, we have found the maxima and minima of the bandwidth at the same points as for the case of standard electrons [4, 7].

4.1. Asymptotic Expression

An asymptotic expression for the bandwidth can be obtained by using the following expression for the Laguerre polynomials in the limit of large n as

$$e^{-u/2} L_n(u) \rightarrow (\pi^2 n u)^{-1/4} \cos \left(2(nu)^{1/2} - \frac{\pi}{4} \right) . \quad (14)$$

Substituting the asymptotic expression given by (14) into (13) yields the asymptotic expression for bandwidth

$$\Delta = V_0 (\pi^2 n u)^{-1/4} \cos \left(\frac{1}{2}(u/n)^{1/2} \right) \cos \left(2(nu)^{1/2} - \frac{\pi}{4} \right) \quad (15)$$

$$= V_0 \left(\frac{a}{\pi^2 R_g} \right)^{\frac{1}{2}} \cos \left(\frac{\pi R_g}{2an} \right) \cos \left(\frac{2\pi R_g}{a} - \frac{\pi}{4} \right), \quad (16)$$

where we have rewritten (15) containing $u = K^2 \ell^2 / 2$ in terms of the ratio of the semi-classical orbital radius R_g and the modulation period a . This expression can be easily understood by analogy with the *beating* of 2 oscillators of similar frequencies: the first cosine term is the amplitude of the beat. This extra modulation of the bandwidth is the most significant difference between the DOS of a normal 2DEG and graphene. Note that for large n it approaches unity as $(u/n)^{-1}$.

For large n the level spacing goes as $\omega_g (n^{1/2} - (n-1)^{1/2}) \rightarrow \omega_g \frac{1}{2} n^{-1/2}$ and the width goes as $(\pi^2 n u)^{-1/4}$, apart from the modulation. There is therefore a value of n at which the width becomes equal to the spacing and the perturbation theory is no longer valid. This occurs when

$$n_{\max} = \frac{1}{16} \pi^2 u \omega_g^4 = \frac{\pi^4}{2a^2 V_0^4} v^4 e B. \quad (17)$$

For a fixed electron density this suggests a minimum value for the magnetic field B below which it is necessary to carry out a more sophisticated analysis. Note that this argument also applies to any other calculation [8] which treats the modulation as a perturbation.

4.2. Classical description

We now give a classical explanation of the asymptotic expression of bandwidth obtained in (16) which is essentially a large n expression. The classical equations of motion along the x and y directions are

$$x(t) = x_0 + R_g \sin(\omega_g t + \varphi) \quad (18a)$$

$$y(t) = y_0 + R_g \cos(\omega_g t + \varphi) \quad (18b)$$

respectively, where R_g is the radius of the orbit, x_0 and y_0 are the centre coordinates and φ is phase factor. Note that this approach is valid for both graphene and parabolic systems apart from the fact that the orbital radius R_g scales as E_F in the graphene case but as $E_F^{1/2}$ otherwise. Without loss of generality we may take $\varphi = 0$. Thus the increase in the average energy of the cyclotron motion due to the electric modulation is evaluated as

$$\Delta E(x_0) = \frac{1}{t_0} \int_{-t_0/2}^{+t_0/2} V_0 \cos(Kx(t)) dt \quad (19)$$

where t_0 is the period of the orbit. This result is valid to the same order as (7). Substituting $x(t)$ yields

$$\Delta E(x_0) = V_0 J_0(K R_g) \cos(K x_0) \quad (20)$$

with $J_0(z)$ the Bessel function of zero order. For $2\pi R_g > a$, one can replace the Bessel function J_0 by a cosine function as

$$J_0 \left(\frac{2\pi R_g}{a} \right) \simeq \left(\frac{a}{\pi^2 R_g} \right)^{\frac{1}{2}} \cos \left(\frac{2\pi R_g}{a} - \frac{\pi}{4} \right) \quad (21)$$

with the result

$$\Delta E(x_0) = V_0 \left(\frac{a}{\pi^2 R_g} \right)^{\frac{1}{2}} \cos \left(\frac{2\pi R_g}{a} - \frac{\pi}{4} \right), \quad (22)$$

which is almost the same as obtained in (16) in the limit of large n . The significant difference between (16) and (22) is the extra cosine factor which has its origin in the mixing between consecutive Landau levels, or Laguerre functions, which is something with no classical equivalent. This reveals itself in (16) in that it has not been possible to rewrite (15) in terms of purely classical quantities: there is a residual n in the extra factor.

5. Conclusions

In this work we have analysed the band spectrum of graphene with a magnetic field perpendicular to the graphene layer and a unidirectional electric modulation. We have determined the density of electronic states and the bandwidth of each level. We have also considered the asymptotic expression for the bandwidth and its relation to a classical description and have noted a quantum correction to the classical behaviour. To highlight the effects of modulation on the density of states and bandwidth, we have plotted these quantities for experimentally relevant parameters.

Acknowledgments

One of us (K.S.) would like to acknowledge the support of the Pakistan Science Foundation (PSF) through project No. C-QU/Phys (129). M. T. would like to acknowledge the support of the Pakistan Higher Education Commission (HEC).

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